

# Tight Binding sp3s\* Material Parameters From Genetic Algorithms

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## Outline:

- Sp3s\* tight binding models essential for electron transport.
- Need 2nd neighbor sp3s\* (or sp3d5) for transport in X, L
- > 37-dimensional parameter fitting problem.
- Get parameter with genetic algorithms.
- Conclusion

# Heterostructure Electron Transport

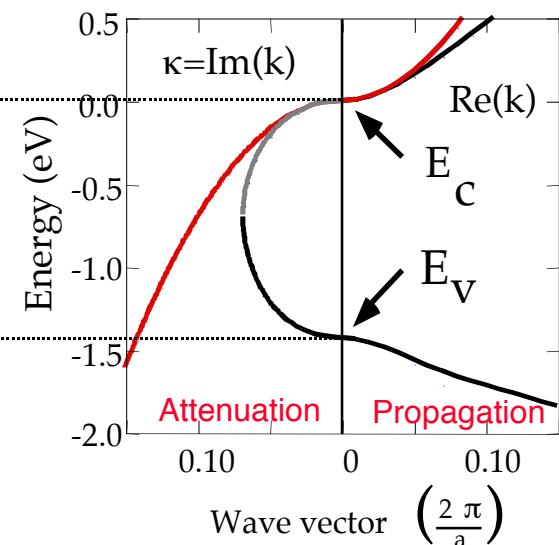
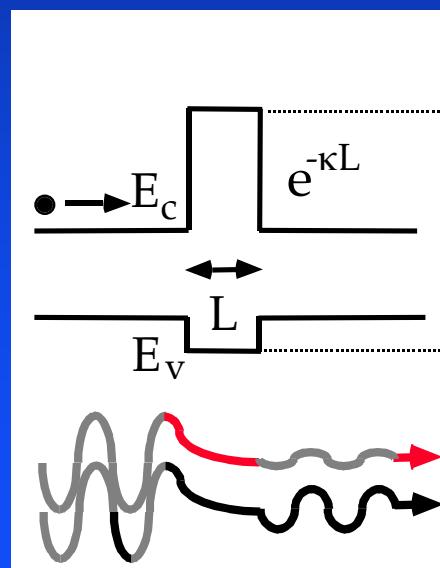
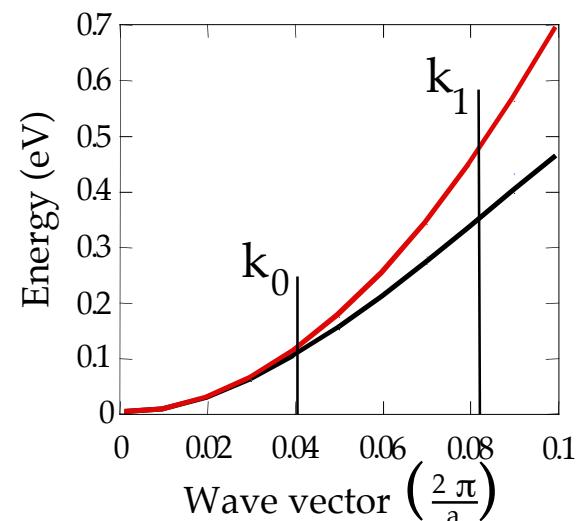
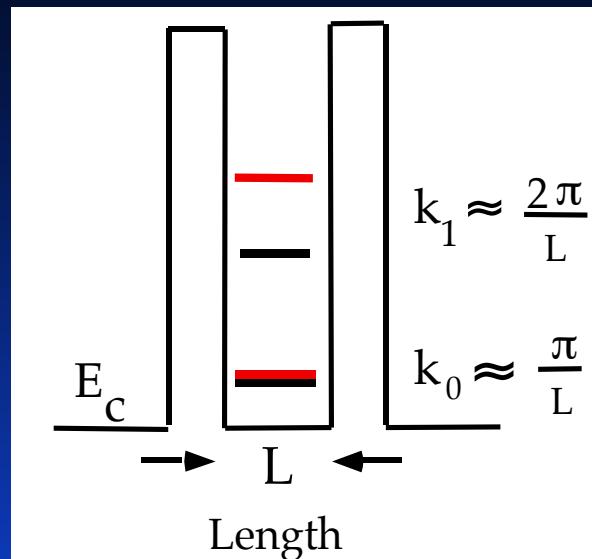
# Need monolayer resolution!

- Parabolic / 1 band
- Non-parabolic / Coupled bands

Non-parabolicity lowers  
second state  
-> Second turn-on at  
lower voltages.

- Band wrapping reduces attenuation  
-> Current increases

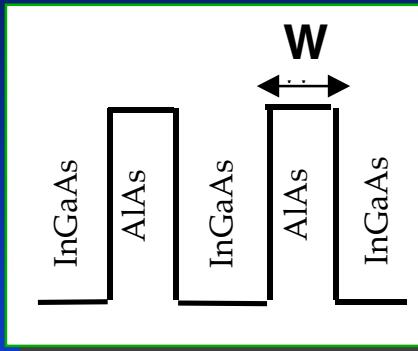
# Tight Binding Models are Essential



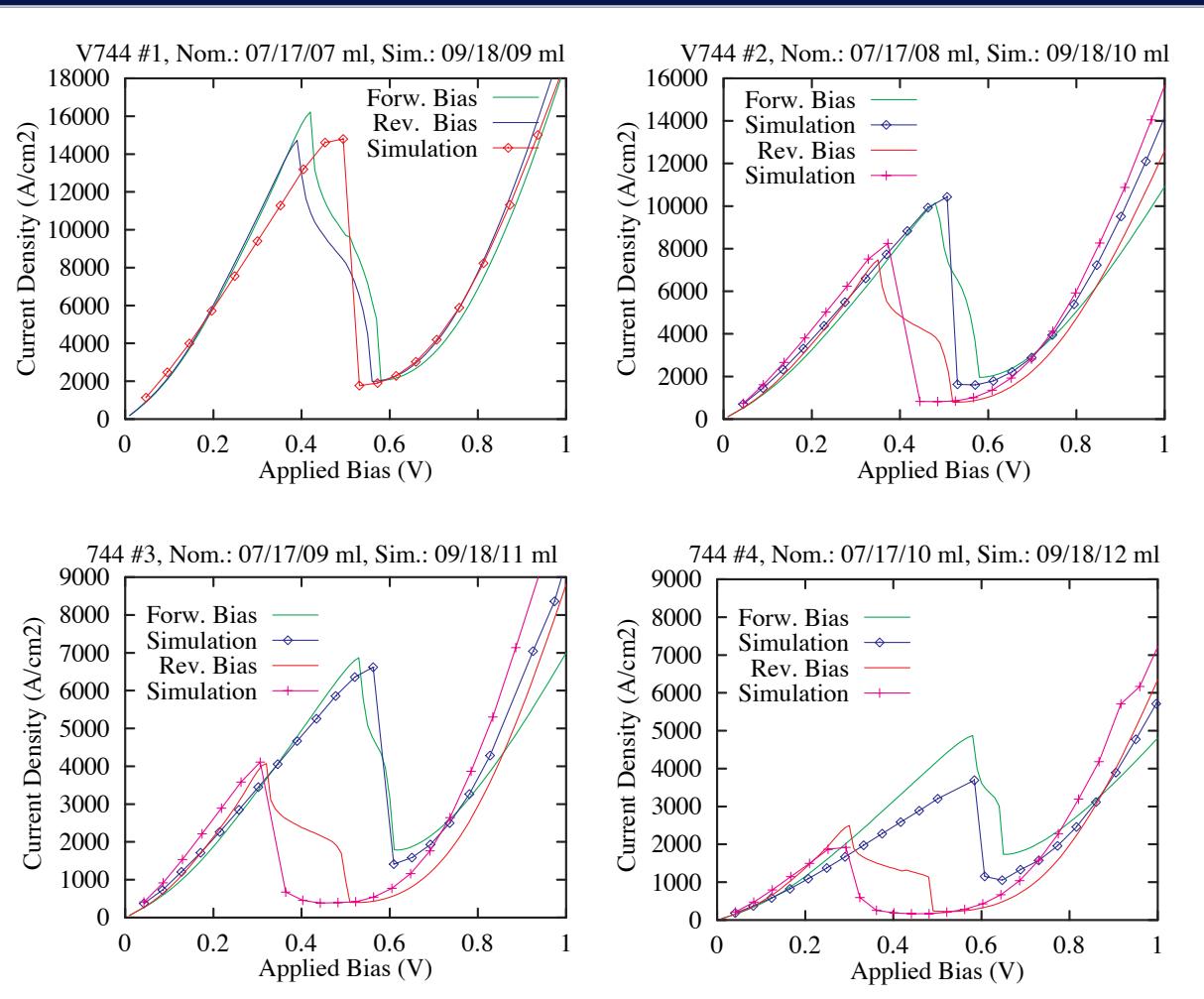
# sp3s\* Success: NEMO Simulation

Strained InGaAs/AlAs 4 Stack RTD with Asymmetric Barrier Variation

**Vary One Barrier Thickness**



**Four increasingly asymmetric devices:**  
**20/50/20 A [1]**  
**20/50/23 A [2]**  
**20/50/25 A [3]**  
**20/50/27 A [4]**

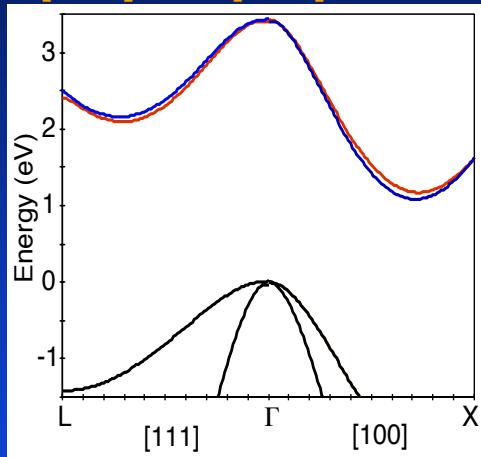


Presented at IEEE DRC 1997, work performed at Texas Instrument, Dallas

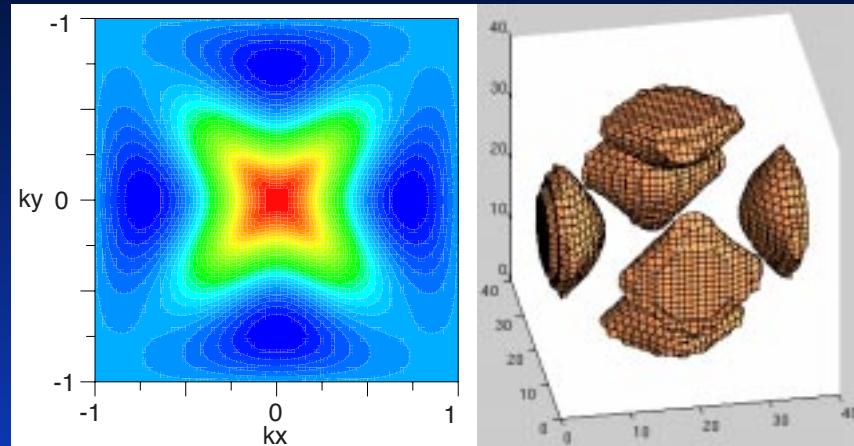
# Transport in X or L Valleys?

Pathology of nearest neighbor sp<sub>3</sub>s\* Model.

Nearest neighbor and  
2nd nearest neighbor sp<sub>3</sub>s\*  
Identical dispersions in  
[100] and [111] for Si

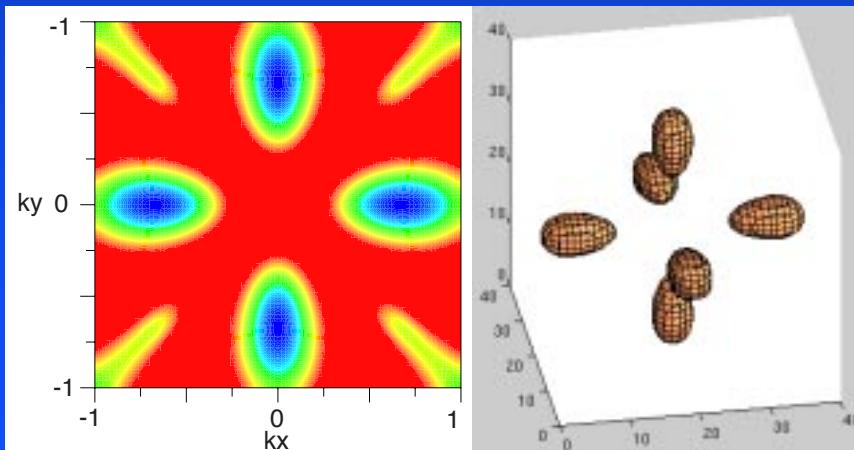


- Si band structure:
  - conduction band minimum at X
  - $m_h = 0.91$     $m_l = 0.19$
- Nearest neighbor sp<sub>3</sub>s\*:
  - $m_h = 0.74$     $m_l = 1.62 \rightarrow \text{infinite}$
- 2nd Nearest neighbor sp<sub>3</sub>s\*:
  - $m_h = 0.68$     $m_l = 0.29$



Nearest neighbor sp<sub>3</sub>s\*      15 parameters

2<sup>nd</sup> Nearest neighbor sp<sub>3</sub>s\*    37 parameters



# Tight Binding Parameter Fitting is Painful !

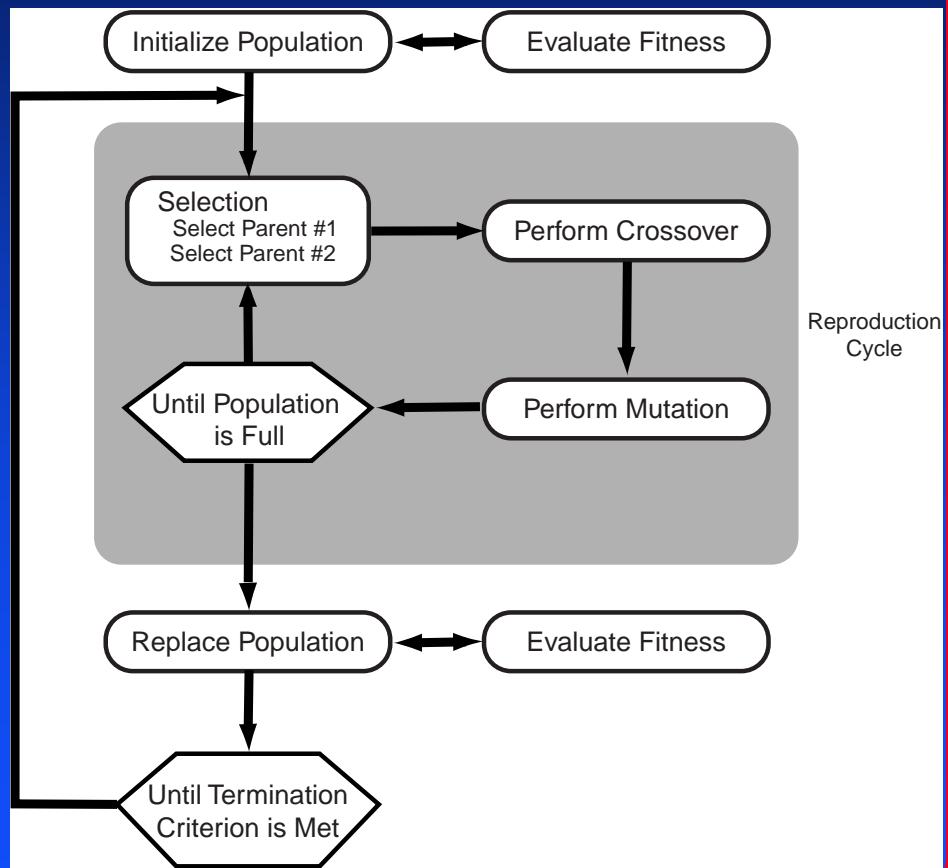
## Problem:

- sp3s\* nearest neighbor model has 15 “free” parameters.
- 2nd nearest neighbor model has 37 “free” parameters.
- No analytic / direct connection in the whole Brillouin zone between
  - orbital interaction energies and
  - band edges, effective masses

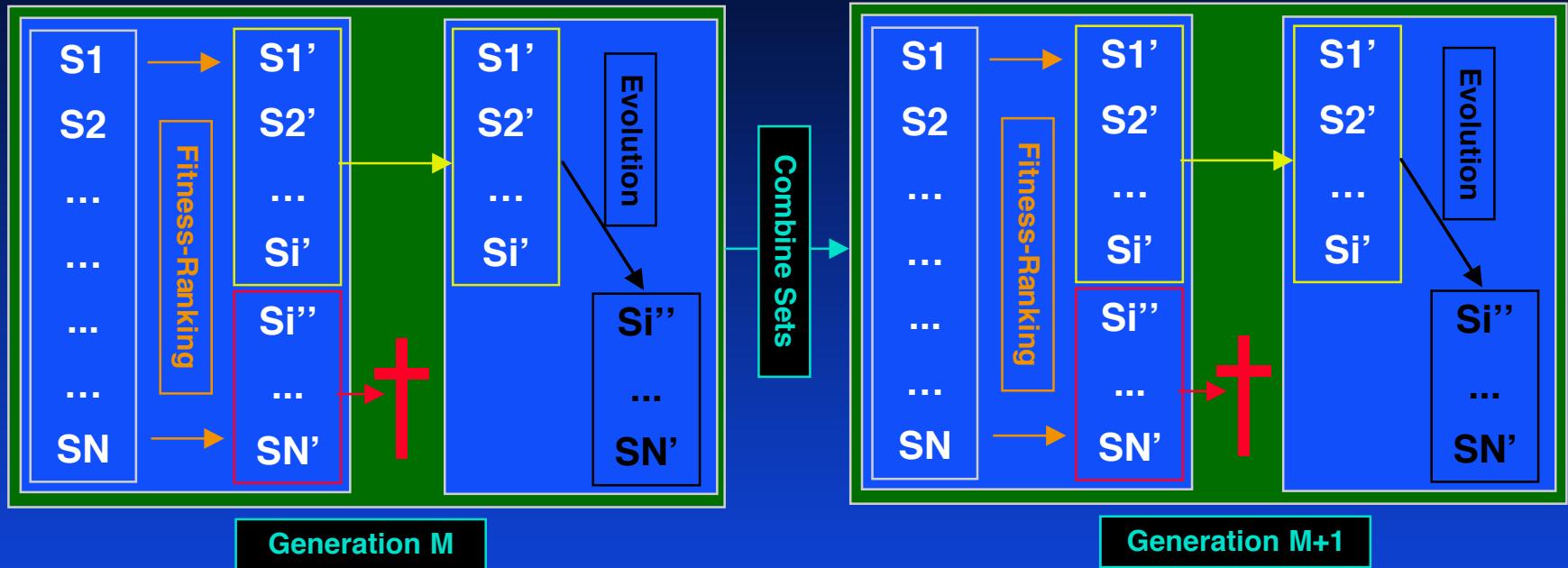
Large-dimensional fitting Problem!!!

## Approach:

### Genetic Algorithm Optimization



# Basic Genetic Algorithm

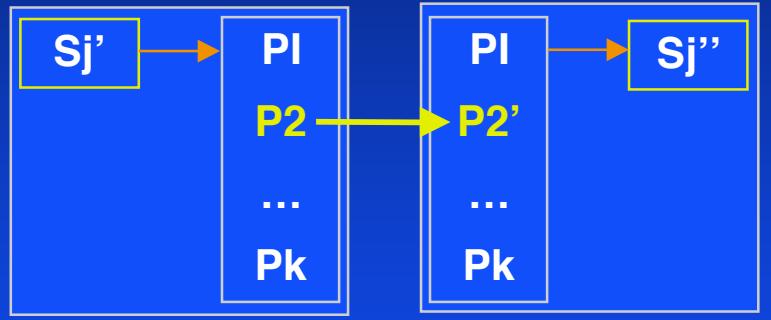


- Genetic algorithm parameter optimization is based on:
  - Survival of good parameter sets
  - Evolution of new parameter sets
  - Survival of a diverse population
- Optimization can be performed globally, rather than locally.

# Basic Evolution Operations

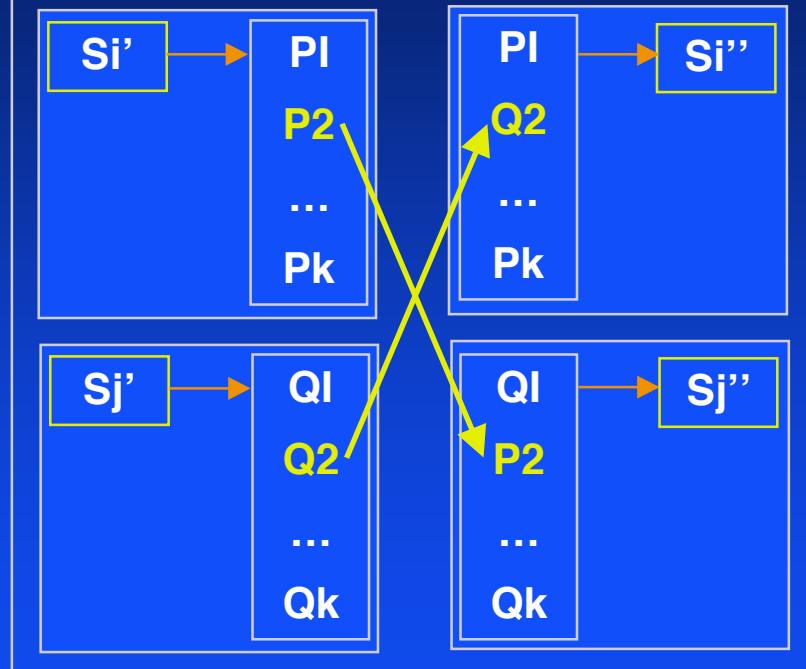
- Each set ( $S_i$ ) consists of several parameters ( $P_j$ )
- The parameters  $P_j$  can be of different kinds: real, integers, symbols, ...

## Mutation operation



- Mutation may move parameters out of their original parameter range
  - E.g: original range [5,6,7,...100]  
5 could be mutated to 4, or 3 ...
- Mutation size may be random.
- Multiple parameters may be mutated at the same step.

## Crossover operation



- Crossover maintains the original parameters range.
- Crossover explores different combinations of existing genes.

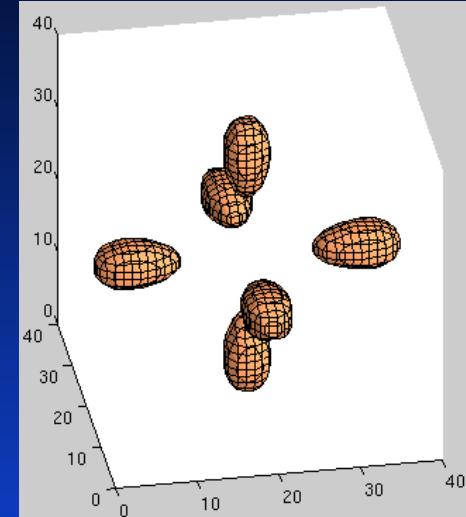
## 2<sup>nd</sup> Nearest Neighbor Model: Optimization in a 37-dimensional Space

Value	Target	Rel. Error	Description
0.0006	0.0000	5.72E-04	Vhh_E
0.6760	0.7500	9.87E-02	kz_X_Delta
<b>1.1330</b>	<b>1.1300</b>	<b>2.62E-03</b>	<b>E_kz_X_Delta</b>
<b>0.8931</b>	<b>0.9163</b>	<b>2.53E-02</b>	<b>mlong_kz_X_Delta</b>
<b>0.1932</b>	<b>0.1905</b>	<b>1.40E-02</b>	<b>mtran_kz_X_Delta</b>
-0.1515	-0.1530	1.00E-02	VIh_mlong_001
-0.5281	-0.5370	1.65E-02	Vhh_mlong_001
-0.2399	-0.2340	2.52E-02	Vso_mlong_001
0.0451	0.0450	3.25E-03	Delta_so
1.5745	1.6000	1.59E-02	E_kz_K_Delta
2.8168	3.3500	1.59E-01	Cgam_Eg
1.7742	2.0500	1.35E-01	E_kz_L_Delta

Value	Target	Rel. Error	Description
0.0001968	0	1.97E-04	Vhh_E
<b>0.664905</b>	<b>0.664</b>	<b>1.36E-03</b>	<b>E_kz_L_Delta</b>
<b>1.575913</b>	<b>1.59</b>	<b>8.86E-03</b>	<b>mlong_kz_L_Delta</b>
<b>0.081305</b>	<b>0.0807</b>	<b>7.50E-03</b>	<b>mtran_kz_L_Delta</b>
-0.04369	-0.0438	2.61E-03	VIh_mlong_001
-0.04232	-0.0426	6.48E-03	VIh_mlong_011
-0.04191	-0.043	2.54E-02	VIh_mlong_111
-0.27446	-0.284	3.36E-02	Vhh_mlong_001
-0.34398	-0.376	8.52E-02	Vhh_mlong_011
-0.37411	-0.352	6.28E-02	Vhh_mlong_111
<b>-0.09513</b>	<b>-0.095</b>	<b>1.40E-03</b>	<b>Vso_mlong_001</b>
0.0393357	0.038	3.51E-02	Cgam_mlong
0.8012496	0.805	4.66E-03	Cgam_Eg
0.8	0.84	4.76E-02	kz_X_Delta
1.1020801	1.16	4.99E-02	E_kz_X_Delta
0.2882422	0.3	3.92E-02	Delta_so

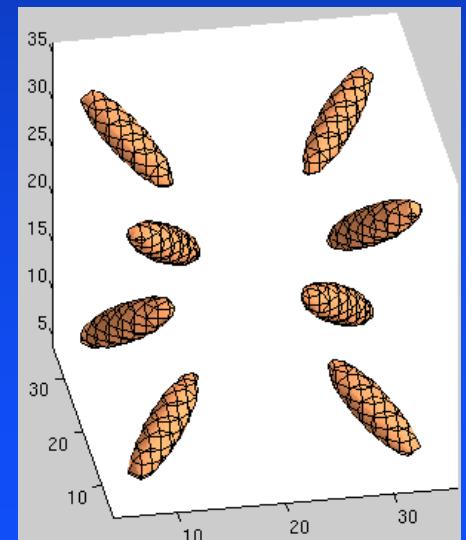
### Si Target:

- Energy at X
- Masses at X
- Hole masses



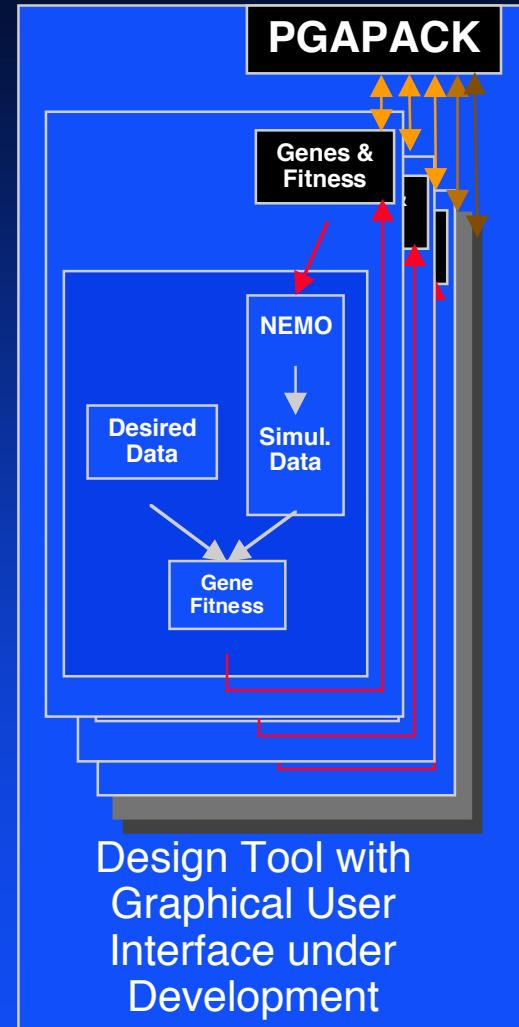
### Ge Target:

- Energy at L
- Masses at L
- Hole masses



## Conclusions and Future Plans

- Massively parallel genetic algorithm enables GLOBAL optimization on large problems.
- Can fit energies and effective masses off the Brillouin zone symmetry points.
- Can incorporate “new” materials into the NEMO database for transport simulation.
- Can incorporate “new” bandstructure models such as sp3d5 and take the agony out of the parameter fitting process.
- Develop general purpose optimization tool which is wrapped around simulators like NEMO or SPICE.



PGAPACK was developed by David Levine - Argonne Natl. Lab.